ROBUST SUMMARY FOR CARBAMATE HYDROCHLORIDE

Summary

Carbamate hydrochloride (F3455.HCl) is a solid which is at least 50% soluble in water. No data are available on its melting point, and boiling point, density, and vapor pressure data are not applicable to this chemical. The product as shipped is a liquid, which contains F3455.HCl (35-51%), water (34-40%), dimethylamine hydrochloride (5-14%), and trimethylguanidine hydrochloride (1-5%). The product as shipped has a boiling point of 105°C, a liquid density of 69.7 lb/ft³ at 23°C, and a vapor pressure of 18 mm Hg at 21°C.

Environmental fate data for F-3455.HCl are generally not available. A review of estimated physical-chemical properties and environmental-fate characteristics based on output from EPIWIN 3.05 modeling software (Syracuse Research Corporation) indicates that F-3455.HCl is unlikely to represent a hazard as a persistent and/or bioaccumulative chemical (See Table 1). When modeled using a Level III fugacity model under a standard scenario of equal emissions to air, water, and soil, F-3455.HCl is expected to partition primarily into soil and water compartments. When dissolved in water at environmental pH, F-3455.HCl is expected to be mostly in an ionized form. Hydrolytic decomposition is not expected to readily transform F-3455.HCl, but F-3455.HCl may be subject to aqueous photolysis. Based on the BIOWIN ultimate survey model, F-3455.HCl, is expected to readily biodegrade.

Table 1: Environmental Fate

Bioaccumulation*	BCF = 3.162	
Biodegradation*	Readily biodegradable	
Fugacity*	Level III Par Air Water Soil Sediments	tition Estimate 0.005 % 45 % 54.9 % 0.08 %
* Modeled data	l .	

No aquatic toxicity information was available on carbamate hydrochloride. Modeling of physical-chemical parameters (i.e., log Kow) and aquatic toxicity was conducted to help provide insight into the behavior in the environment and the aquatic toxicity of F3455.HCl (See Table 2). Syracuse Research Corporation models for estimating physical-chemical properties were used to estimate log₁₀ Kow (Meylan and Howard, 1995) for subsequent use in the ECOSAR program. ECOSAR (Meylan and Howard, 1999) was used to estimate aquatic toxicity data for green algae, daphnids (planktonic freshwater crustaceans), and fish. ECOSAR predictions are based on actual toxicity test data for classes of compounds with similar modes of action. The predicted

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log₁₀ Kow value was used as input for the ECOSAR model (see Table 2 for value). The ECOSAR predictions indicate that F3455.HCl is unlikely to be acutely toxic to algae, invertebrates, or fish at environmentally relevant concentrations. Since there are no analog chemicals with existing test data to lend support to the modeled data, acute toxicity screening tests are proposed with fish, *Daphnia*, and algae.

Table 2: Predicted Aquatic Toxicity Values

Parameter	Estimated Value
Log Kow	-0.07 @ 25°C
96-hour LC ₅₀ (fish)	11,334 mg/L
48-hour EC ₅₀ (daphnid)	10,527 mg/L
96-hour EC ₅₀ (green algae)	5842 mg/L

The product as shipped has very low acute oral toxicity with an acute lethal dose (ALD) > 11,000 mg/kg in rats. Lethargy was observed on the day of dosing in animals administered 7500 and 11,000 mg/kg. Slight initial weight loss was evident at 670, 1500, 3400, 7500, and 11,000 mg/kg. No data regarding developmental and genetic toxicity was found. Therefore, a developmental study, *in vitro* bacterial reverse mutation assay, and *in vitro* clastogenicity study in human peripheral blood lymphocytes following OECD guidelines 414, 471, and 473, respectively are proposed. As described below, the test material is a closed system intermediate; therefore, repeated dose and reproductive toxicity endpoints are not required.

Human Exposure Information

F3455.HCl is manufactured at the DuPont Belle Plant and shipped to the DuPont LaPorte Plant. DuPont LaPorte is the only customer. The sites can have from 2 to 10 personnel working (construction, contractor, and plant employees) in the F3455.HCl operating areas. The areas where the substance is manufactured will have 2 operators present per shift during normal operations and 5 to 10 people during a shutdown or major construction activity.

The F3455.HCl is not present in the distributed product. There are a series of chemical reaction steps, and the F3455.HCl is consumed by chemical reaction. Chemical analysis of the product sold in commerce shows no detectable amount. The detection limit is estimated to be 0.1 wt% based on liquid chromatography.

Transport between the two locations is via dedicated rail cars or trucks. The F3455.HCl is shipped in bulk as the hydrochloride salt in water. Annual volume is 2.5-3 million pounds transported.

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Controls during transport and transfer at the dispatching and receiving site are designed to ensure a closed system. This solution is pumped directly from the reactor to the railcar or truck for shipment. Normal shipment is by railcar. During loading of the railcar, the railcar dome is vented to the atmosphere. Because the aqueous salt solution has a low vapor pressure, the only significant exposure risk is as a result of a spill during loading of the railcar or truck. For railcars, spill containment including a stainless steel catch pan with a double-lined sump is provided for spill protection. Railcars are inspected to maintain the integrity of the fleet. The bottom valve of tank cars or trucks is checked by DuPont Belle operators when loading first starts (plug is removed to look for any liquid that may have leaked through the valve). The operator who loads the car wears appropriate PPE to guard against splashes. A checklist is completed for each shipment, to ensure that standard procedures are followed. Any spills, water used to wash equipment, etc., is sent to the biological treatment system on-site.

On receipt of the product at DuPont LaPorte, the solution is again handled in a closed system that includes pumping from the railcar or truck to the storage tank. It is consumed in the manufacturing process in a closed pipe and reactor system. The only significant exposure risk is during the unloading operation. The unloading spot is equipped with spill containment (catch pan) and the storage tank is diked. Any spills in these containment areas are disposed of by on-site incineration or biological treatment. Both the unloading spot and the storage tank vent to a flare. Unloading operators or others that might perform first breaks into equipment wear PPE to guard against splashes.

References for the Summary

Meylan, W. M. and P. H. Howard (1995). J. Pharm. Sci., 84:83-92.

Meylan, W. M. and P. H. Howard (1999). <u>User's Guide for the ECOSAR Class Program</u>, Version 0.993 (Mar 99), prepared for J. Vincent Nabholz and Gordon Cas, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, DC, prepared by Syracuse Research Corp., Environmental Science Center, Syracuse, NY 13210 (submitted for publication).